

Welcome to STN International! Enter x:x

LOGINID:sssptaul2lbd

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

10/035005

* * * * * Welcome to STN International * * * * *

NEWS 1 Web Page URLs for STN Seminar Schedule - N. America
NEWS 2 Apr 08 "Ask CAS" for self-help around the clock
NEWS 3 Apr 09 BEILSTEIN: Reload and Implementation of a New Subject Area
NEWS 4 Apr 09 ZDB will be removed from STN
NEWS 5 Apr 19 US Patent Applications available in IFICDB, IFIPAT, and IFIUDB
NEWS 6 Apr 22 Records from IP.com available in CAPLUS, HCAPLUS, and ZCAPLUS
NEWS 7 Apr 22 BIOSIS Gene Names now available in TOXCENTER
NEWS 8 Apr 22 Federal Research in Progress (FEDRIP) now available
NEWS 9 Jun 03 New e-mail delivery for search results now available
NEWS 10 Jun 10 MEDLINE Reload
NEWS 11 Jun 10 PCTFULL has been reloaded
NEWS 12 Jul 02 FOREGE no longer contains STANDARDS file segment
NEWS 13 Jul 22 USAN to be reloaded July 28, 2002;
saved answer sets no longer valid
NEWS 14 Jul 29 Enhanced polymer searching in REGISTRY
NEWS 15 Jul 30 NETFIRST to be removed from STN
NEWS 16 Aug 08 CANCERLIT reload
NEWS 17 Aug 08 PHARMAMarketLetter(PHARMAML) - new on STN
NEWS 18 Aug 08 NTIS has been reloaded and enhanced
NEWS 19 Aug 19 Aquatic Toxicity Information Retrieval (AQUIRE)
now available on STN
NEWS 20 Aug 19 IFIPAT, IFICDB, and IFIUDB have been reloaded
NEWS 21 Aug 19 The MEDLINE file segment of TOXCENTER has been reloaded
NEWS 22 Aug 26 Sequence searching in REGISTRY enhanced
NEWS 23 Sep 03 JAPIO has been reloaded and enhanced
NEWS 24 Sep 16 Experimental properties added to the REGISTRY file
NEWS 25 Sep 16 Indexing added to some pre-1967 records in CA/CAPLUS
NEWS 26 Sep 16 CA Section Thesaurus available in CAPLUS and CA
NEWS 27 Oct 01 CASREACT Enriched with Reactions from 1907 to 1985
NEWS 28 Oct 21 EVENTLINE has been reloaded

NEWS EXPRESS October 14 CURRENT WINDOWS VERSION IS V6.01,
CURRENT MACINTOSH VERSION IS V6.0a(ENG) AND V6.0Ja(JP),
AND CURRENT DISCOVER FILE IS DATED 01 OCTOBER 2002
NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS INTER General Internet Information
NEWS LOGIN Welcome Banner and News Items
NEWS PHONE Direct Dial and Telecommunication Network Access to STN
NEWS WWW CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 09:43:32 ON 22 OCT 2002

=> fil reg

FILE 'REGISTRY' ENTERED AT 09:43:47 ON 22 OCT 2002

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 21 OCT 2002 HIGHEST RN 463926-32-1

DICTIONARY FILE UPDATES: 21 OCT 2002 HIGHEST RN 463926-32-1

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STN Note 27, Searching Properties in the CAS Registry File, for complete details:

<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

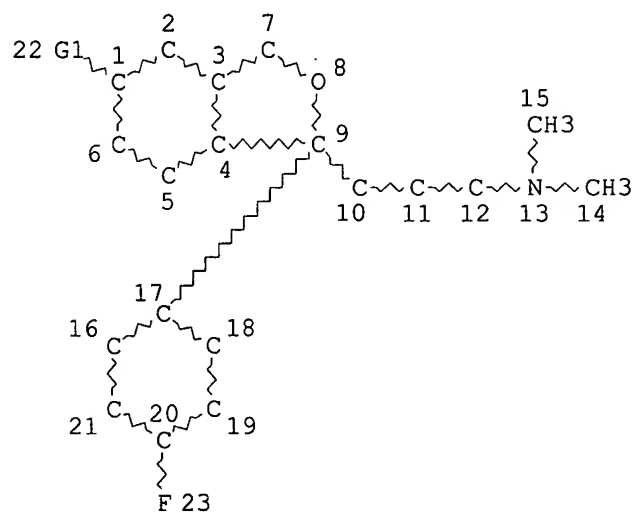
*** YOU HAVE NEW MAIL ***

'REGISTRY' IS DEFAULT FORMAT FOR 'REGISTRY' FILE

=> d sia

L1 HAS NO ANSWERS

L1 STR



VAR G1=COOH/CN

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 23

STEREO ATTRIBUTES: NONE

=> s l1 fu

COMBINATION OF STRUCTURE AND TEXT TERMS NOT VALID

The query entered contains both search terms created by structure-building or screen commands and text search terms. L#s created via the STRUCTURE or SCREEN commands must be searched in the structures files separately from text terms or profiles. The L# answer sets from structure searches can be used in crossover searches and can be combined with text terms.

=>

=> s l1

SAMPLE SEARCH INITIATED 09:49:26 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 9 TO ITERATE

100.0% PROCESSED 9 ITERATIONS

2 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 9 TO 360

PROJECTED ANSWERS: 2 TO 124

L2 2 SEA SSS SAM L1

=> s l1 ful

FULL SEARCH INITIATED 09:49:40 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 157 TO ITERATE

100.0% PROCESSED 157 ITERATIONS

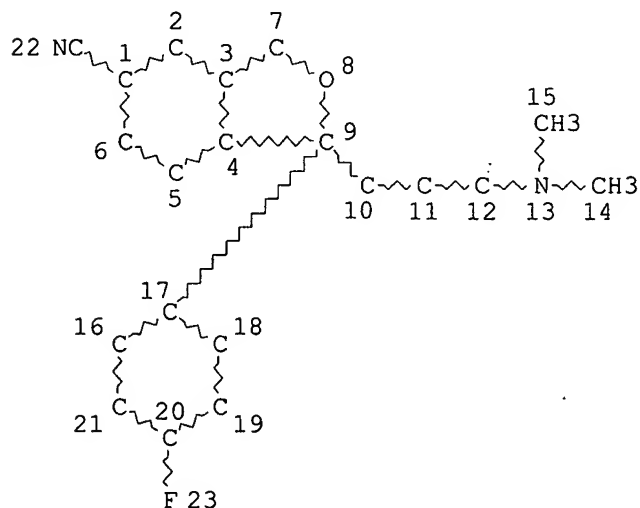
31 ANSWERS

SEARCH TIME: 00.00.02

L3 31 SEA SSS FUL L1

=> str l1

:nod 22 cn,dis



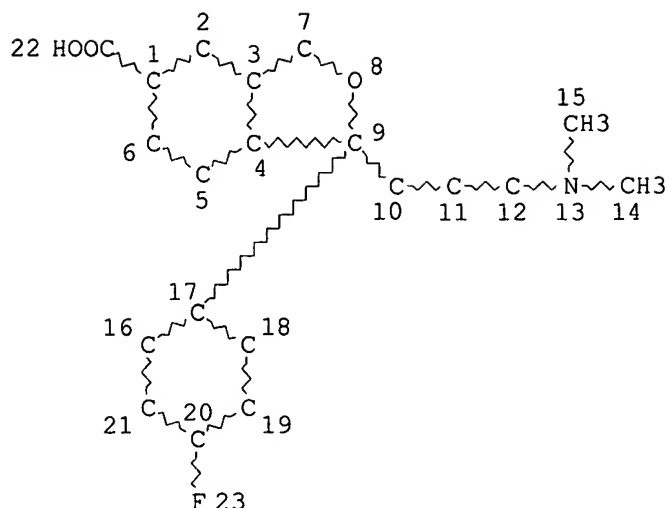
:end

L4 STRUCTURE CREATED

=> str l1

:nod 22 cooh

:dis



:end

L5 STRUCTURE CREATED

=> search 14

ENTER TYPE OF SEARCH (SSS), CSS, FAMILY, OR EXACT:.
 ENTER SCOPE OF SEARCH (SAMPLE), FULL, RANGE, OR SUBSET:sub
 ENTER SUBSET L# OR (END):13
 ENTER SUBSET SEARCH SCOPE - SAMPLE, FULL, RANGE, OR (END):ful
 FULL SUBSET SEARCH INITIATED 09:51:24 FILE 'REGISTRY'
 FULL SUBSET SCREEN SEARCH COMPLETED - 28 TO ITERATE

100.0% PROCESSED 28 ITERATIONS 28 ANSWERS
 SEARCH TIME: 00.00.01

L6 28 SEA SUB=L3 SSS FUL L4

=> search 15

ENTER TYPE OF SEARCH (SSS), CSS, FAMILY, OR EXACT:.
 ENTER SCOPE OF SEARCH (SAMPLE), FULL, RANGE, OR SUBSET:sub
 ENTER SUBSET L# OR (END):13
 ENTER SUBSET SEARCH SCOPE - SAMPLE, FULL, RANGE, OR (END):ful
 FULL SUBSET SEARCH INITIATED 09:51:50 FILE 'REGISTRY'
 FULL SUBSET SCREEN SEARCH COMPLETED - 31 TO ITERATE

100.0% PROCESSED 31 ITERATIONS 3 ANSWERS
 SEARCH TIME: 00.00.01

L7 3 SEA SUB=L3 SSS FUL L5

=> fil caplus

FILE 'CAPLUS' ENTERED AT 09:52:11 ON 22 OCT 2002
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FILE COVERS 1907 - 22 Oct 2002 VOL 137 ISS 17
FILE LAST UPDATED: 21 Oct 2002 (20021021/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

=> s 17

L8 4 L7

=> d tot cbib abs hitstr

L8 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2002 ACS

2002:550142 Document No. 137:78853 Preparation of Citalopram from 5-halo-1-(4-fluorophenyl)-1-(3-dimethylaminopropyl)-1,3-dihydroisobenzofuran.. Petersen, Hans; Ahmadian, Haleh (H. Lundbeck A/S, Den.). Patentschrift (Switz.) CH 691969 A 20011215, 15 pp. (German). CODEN: SWXXAS. APPLICATION: CH 2001-1522 20010816. PRIORITY: DK 2000-1231 20000818.

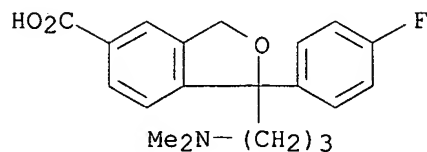
AB Citalopram (I) was prepd. by converting a 5-halo-1-(4-fluorophenyl)-1-(3-dimethylaminopropyl)-1,3-dihydroisobenzofuran to the 5-carboxylic acid deriv. and converting the latter to I. Thus, 5-bromo-1-(4-fluorophenyl)-1-(3-dimethylaminopropyl)-1,3-dihydroisobenzofuran in Me3COMe at -78.degree. was treated with BuLi followed by stirring for 2 h at -30.degree.. Solid CO2 was added followed by stirring for 16 h at room temp. to give 5-carboxy-1-(4-fluorophenyl)-1-(3-dimethylaminopropyl)-1,3-dihydroisobenzofuran. The latter was heated with sulfamide and SOCl2 in sulfolane at 130.degree. for 2 h to give I.

IT 440121-09-5P

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of Citalopram from 5-halo-1-(4-fluorophenyl)-1-(3-dimethylaminopropyl)-1,3-dihydroisobenzofuran)

RN 440121-09-5 CAPLUS

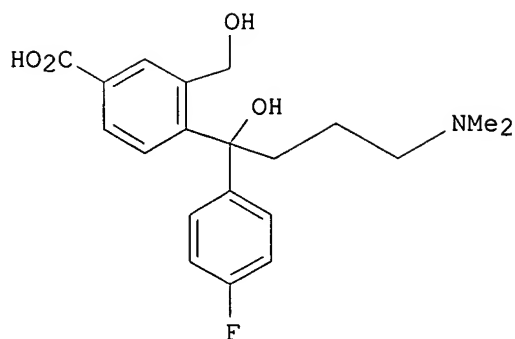
CN 5-Isobenzofurancarboxylic acid, 1-[3-(dimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro- (9CI) (CA INDEX NAME)



L8 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2002 ACS

2002:550141 Document No. 137:78852 Preparation of citalopram from 5-carboxyphthalide and Grignard derivatives of 4-halo-1-fluorobenzenes and 3-dimethylaminopropyl halides.. Dancer, Robert; Petersen, Hans; Ahmadian, Haleh (H. Lundbeck A/S, Den.). Patentschrift (Switz.) CH 691968 A 20011215, 11 pp. (German). CODEN: SWXXAS. APPLICATION: CH 2001-1521 20010816. PRIORITY: DK 2000-1231 20000818.

GI



II

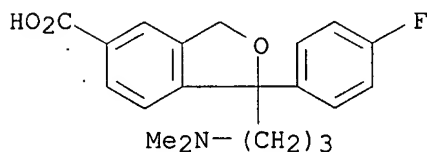
AB Citalopram (I) was prepd. by reaction of 5-carboxyphthalide and Grignard derivs. of 4-halofluorobenzenes and 3-dimethylaminopropyl halides to give diol intermediate (II) followed by cyclization of II and conversion of the resulting carboxycitalopram to I. Thus, 5-carboxyphthalide in THF was treated sequentially with tetramethylethylenediamine, p-fluorophenylmagnesium bromide and MgBr₂ in THF, and 3-dimethylaminopropylmagnesium bromide in THF/heptane to give 5-carboxycitalopram of >80% purity. The latter was heated with sulfamide and SOCl₂ in sulfolane for 2 h at 130.degree. to give citalopram of >97% purity.

IT **440121-09-5P**

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of citalopram from 5-carboxyphthalide and Grignard derivs. of 4-halofluorobenzenes and 3-dimethylaminopropyl halides)

RN 440121-09-5 CAPLUS

CN 5-Isobenzofurancarboxylic acid, 1-[3-(dimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro- (9CI) (CA INDEX NAME)



L8 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2002 ACS

2002:286699 Document No. 136:309841 Process for preparing citalopram and intermediates therefor. Gao, Wei-Guo; Ikemoto, Tetsuya; Iki, Masami (Sumika Fine Chemicals Co., Ltd., Japan). Jpn. Kokai Tokkyo Koho JP 2002114770 A2 20020416, 35 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 2000-302690 20001002.

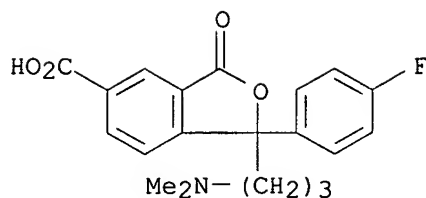
AB Citalopram, a known antidepressant, was prepd. in a multistep process. Thus, 6-carboxy-3-(4'-fluorophenyl)phthalide was converted in 3 steps to 6-cyano-3-(4'-fluorophenyl)phthalide (I). I was converted to 5-cyano-2-(4'-fluorobenzoyl)benzoic acid (II); reaction of II with 3-(dimethylamino)propylmagnesium chloride, followed by redn., gave citalopram.

IT **411221-54-0P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(process for prepg. citalopram and intermediates therefor)

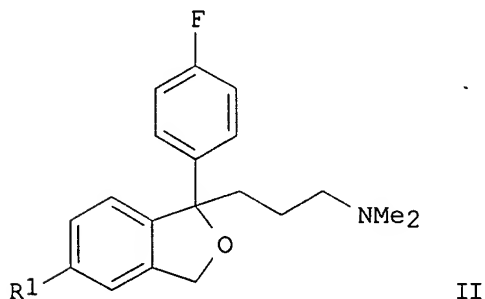
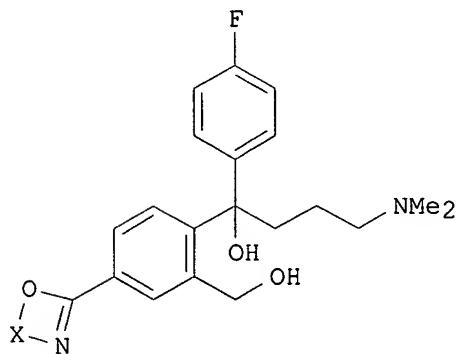
RN 411221-54-0 CAPLUS

CN 5-Isobenzofurancarboxylic acid, 1-[3-(dimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro-3-oxo- (9CI) (CA INDEX NAME)



L8 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2002 ACS
 2001:676759 Document No. 135:242130 Process for the preparation of
 citalopram from diaryl oxazolinediols.. Greenwood, Alan Kenneth;
 McHattie, Derek; Rechka, Josef Antonin; Hedger, Paul Christopher Markus;
 Gamble, Mark Philip (Resolution Chemicals Limited, UK). PCT Int. Appl. WO
 2001066536 A1 20010913, 49 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT,
 AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM,
 DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG,
 KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ,
 NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA,
 UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT,
 BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE,
 IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN:
 PIXXD2. APPLICATION: WO 2001-GB994 20010307. PRIORITY: GB 2000-5477
 20000307.

GI



AB Citalopram was prepd. by (a) converting compds. [I; X = (substituted) C1-6
 alkylene] to compds. (II; R1 = CO₂H or salts or esters thereof), and (b)
 conversion of II to citalopram. Thus, oxazoline diol (III) (prepn. given)
 in pyridine was treated with SOCl₂ and then with POCl₃ followed by 4 h
 stirring to give 48% citalopram.

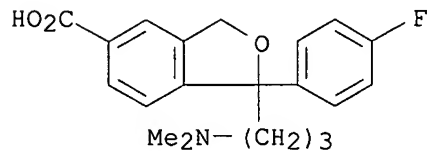
IT 359861-72-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)

(prepn. of citalopram from diaryl oxazolidinediols)

RN 359861-72-6 CAPLUS

CN 5-Isobenzofurancarboxylic acid, 1-[3-(dimethylamino)propyl]-1-(4-
fluorophenyl)-1,3-dihydro-, sodium salt (9CI) (CA INDEX NAME)



=> d his

(FILE 'HOME' ENTERED AT 09:43:32 ON 22 OCT 2002)

FILE 'REGISTRY' ENTERED AT 09:43:47 ON 22 OCT 2002

L1 STR
L2 2 S L1
L3 31 S L1 FUL
L4 STR L1
L5 STR L1
L6 28 SEARCH L4 SUB=L3 FUL
L7 3 SEARCH L5 SUB=L3 FUL

FILE 'CAPLUS' ENTERED AT 09:52:11 ON 22 OCT 2002

L8 4 S L7

=> s distil

L9 4318 DISTIL

=> s l6 and l9

1030 L6
L10 0 L6 AND L9

=> log h

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	23.54	235.07
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-2.48	-2.48

SESSION WILL BE HELD FOR 60 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 09:58:29 ON 22 OCT 2002
Connection closed by remote host